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Mathematical Quantum Mechanics 2
(aka. Mathematical Methods in Quantum Mechanics 2)
7. Homework

Exercise 16

Let V be self-adjoint on G and compact. Consider the Lieb-Thirring inequality

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes G}\big((P^2\otimes \mathbf{1}+V)_-^\gamma\big) \leqslant C^{op}_{\gamma,d}L^{cl}_{\gamma,d}\int_{\mathbb{R}^d}\operatorname{tr}_G\big(V_-^{\gamma+\frac{d}{2}}\big)\,dx, \tag{1}$$

with optimal constant $C^{op}_{\gamma,d}L^{cl}_{\gamma,d}$, where $L^{cl}_{\gamma,d}$ is the (fixed) classical Lieb-Thirring constant. Assume the following three properties:

$$C^{op}_{\gamma,d} \leqslant C^{op}_{\gamma,n}C^{op}_{\gamma+\frac{n}{2},d-n} \quad \forall 1\leqslant n\leqslant d-1, \qquad \text{(Submultiplicativity)} \tag{2}$$

$$1 \leqslant C^{op}_{\gamma_1,d} \leqslant C^{op}_{\gamma_2,d} \quad \forall \gamma_1 \geqslant \gamma_2, \qquad \text{(Monotonicity)} \tag{3}$$

$$C^{op}_{\frac{3}{2},1} = 1, \qquad \text{(Exact value).} \tag{4}$$

Show that

$$C^{op}_{0,d} \leqslant C^{op}_{0,n} \quad \forall d > n \geqslant 3.$$

Solution: From the monotonicity in γ and the exact value for $\gamma = \frac{3}{2}, d = 1$, we infer

$$1 \leqslant C^{op}_{\gamma,1} \leqslant C^{op}_{\frac{3}{2},1} = 1, \quad \forall \gamma \geqslant \frac{3}{2}.$$

Thus if $\gamma \geqslant \frac{3}{2}$ by the submultiplicaticity and monotonicity e.g. for $d = 2$,

$$1 \leqslant C^{op}_{\gamma,2} \leqslant C^{op}_{\gamma,1}C^{op}_{\gamma+\frac{n}{2},1} \leqslant \big(C^{op}_{\gamma,1}\big)^2 = 1,$$

and hence inductively

$$C^{op}_{\gamma,d} = 1 \quad \forall d \in \mathbb{N}, \gamma \geqslant \frac{3}{2}.$$

But then again by the submultiplicaticity, if $d > n \geqslant 3$,

$$C^{op}_{0,d} \leqslant C^{op}_{0,n}C^{op}_{\frac{n}{2},d-n} \leqslant C^{op}_{0,n},$$

which shows the assertion.

Exercise 17

Given V such that $(P^2+V)_- \in \mathcal{S}^1(\mathcal{H})$, and $\sigma_{ess}(P^2+V) \subset [0,\infty)$, show that

$$-\operatorname{tr}\big((P^2+V)_-\big) = \inf_{\sigma\in\mathcal{S}^1, 0\leqslant\sigma\leqslant 1} \operatorname{tr}(\sigma(P^2+V)), \tag{5}$$

where $0 \leqslant \sigma \leqslant 1$ is understood in the sense that $\sigma = \sum_{j\in\mathbb{N}} \lambda_j |\varphi_j\rangle\langle\varphi_j|$ for some orthonormal family $(\varphi_j)_j$ in $\mathcal{H}$, and $0 \leqslant \lambda_j \leqslant 1$, $\sum_{j=1}^\infty \lambda_j < \infty$.

Solution: We prove $\geqslant$ in (5). Since $\sigma_{ess}(P^2+V) \subset [0,\infty)$ we see that given the normalized eigenvectors of $H = P^2 + V$,

$$H\psi_j = E_j\psi_j,$$

we may write

$$H_- = \sum_j E_j \left|\psi_j\right\rangle \left\langle\psi_j\right|.$$

Thus choosing $\sigma = \sum_j \left|\psi_j\right\rangle \left\langle\psi_j\right|$ we see

$$\operatorname{tr}(\sigma H) = \operatorname{tr}\Big(\sum_j \left|\psi_j\right\rangle \left\langle\psi_j\right| H\Big) = \operatorname{tr}\Big(\sum_j E_j \left|\psi_j\right\rangle \left\langle\psi_j\right|\Big) = \sum_j E_j = \operatorname{tr}(H_-).$$

We turn to the inequality $\leqslant$. Take

$$\sigma = \sum_{j\in\mathbb{N}} \lambda_j \left|\varphi_j\right\rangle \left\langle\varphi_j\right|,$$

where $(\varphi_j)_j$ is an orthonormal family in $\mathcal{H}$, $0 \leqslant \lambda_j \leqslant 1$, $\sum_{j=1}^{\infty} \lambda_j < \infty$. We extend φ_k to an orthonormal system by adding $\tilde{\varphi}_k$ to the family. Then, using the orthonormality of φ_j,

$$\begin{aligned}
\operatorname{tr}(\sigma H) &= \sum_k \left\langle\varphi_k\right| \sigma H \left|\varphi_k\right\rangle + \sum_k \left\langle\tilde{\varphi}_k\right| \sigma H \left|\tilde{\varphi}_k\right\rangle \\
&= \sum_{k,j} \lambda_j \left\langle\varphi_k\right| \left|\varphi_j\right\rangle \left\langle\varphi_j\right| H \left|\varphi_k\right\rangle + \sum_{k,j} \lambda_j \left\langle\tilde{\varphi}_k\right| \left|\varphi_j\right\rangle \left\langle\varphi_j\right| H \left|\tilde{\varphi}_k\right\rangle \\
&= \sum_k \lambda_k \left\langle\varphi_k\right| H \left|\varphi_k\right\rangle
\end{aligned}$$

We split $H = H_- + H_+ = \sum_i E_i \left|\psi_i\right\rangle \left\langle\psi_i\right| + H_+$, where H_+ is positive semidefinite, and find

$$\begin{aligned}
\operatorname{tr}(\sigma H) &= \sum_{k,i} E_i\lambda_k \left\langle\varphi_k\right| \left|\psi_i\right\rangle \left\langle\psi_i\right| \left|\varphi_k\right\rangle + \sum_k \lambda_k \left\langle\varphi_k\right| H_+ \left|\varphi_k\right\rangle \\
&\geqslant \sum_{k,i} E_i\lambda_k \left\langle\varphi_k\right| \left|\psi_i\right\rangle \left\langle\psi_i\right| \left|\varphi_k\right\rangle \\
&= \sum_{k,i} E_i\lambda_k \left| \left\langle\varphi_k\right| \left|\psi_i\right\rangle \right|^2 \\
&\geqslant \sum_{k,i} E_i \left| \left\langle\varphi_k\right| \left|\psi_i\right\rangle \right|^2 \\
&\geqslant \sum_i E_i,
\end{aligned}$$

where in the second last inequality we used $0 \leqslant \lambda_k \leqslant 1$, and in the last inequality Parseval, that is $\sum_k \left| \left\langle\varphi_k\right| \left|\psi_i\right\rangle \right|^2 \leqslant 1$ from normality of ψ_i, φ_k.

Exercise 18

Consider a non-negative, convex function $G : \mathbb{R}_+ \to \mathbb{R}_+$ and define its Legendre transformation as

$$G(s) = \sup_{t\geqslant 0}(st - F(t)).$$

Prove that the following are equivalent:

- The Lieb-Thirring bound

$$\operatorname{tr}\big((P^2+V)_-\big) \leqslant \int_{\mathbb{R}^d} G(V_-(x))\,dx, \tag{6}$$

- The Thomas-Fermi bound

$$\langle \psi, \sum_{n=1}^{N} P^2 \psi\rangle_{\Lambda^N L^2(\mathbb{R}^d)} \geqslant \int_{\mathbb{R}^d} F(\varrho_\psi(x))\,dx, \tag{7}$$

  for all $\psi \in \Lambda^N L^2(\mathbb{R}^d)$ with norm one, and where

$$\varrho_\psi(x) = N \int_{\mathbb{R}^{(N-1)d}} |\psi(x, x_2, \ldots, x_N)|^2\,dx_2 \ldots dx_N.$$

Solution: See proof of Theorem 1 in the below excerpt of the paper *Hundertmark, Dirk. Some bound state problems in quantum mechanics. Spectral theory and mathematical physics: a Festschrift in honor of Barry Simon's 60th birthday, 463-496, Proc. Sympos. Pure Math., 76, Part 1, Amer. Math. Soc., Providence, RI, 2007*

Thus

$$\lim_{\lambda\to\infty} \lambda^{-(\gamma+d/2)} S^\gamma(\lambda V) = \frac{1}{(2\pi)^d} \iint (|\xi|^2 + V(x))_-^\gamma \, d\xi dx \\ = L^{\mathrm{cl}}_{\gamma,d} \int V(x)_-^{\gamma+d/2} \, dx. \tag{14}$$

Of course, to make this sketch rigorous, one needs to handle the error terms more carefully, which we skip. This large coupling asymptotic shows that the best possible constants $L_{\gamma,d}$ in the Lieb-Thirring inequality have the natural lower bound $L_{\gamma,d} \geq L^{\mathrm{cl}}_{\gamma,d}$, or, equivalently, $C_{\gamma,d} \geq 1$.

1.5. **A Sobolev inequality for fermions.** Besides being mathematically very appealing, the $\gamma = 1$ version of the Lieb-Thirring bound gives a Sobolev inequality for fermions whose $d = 3$ version has a nice application to the Stability-of-Matter problem. For notational simplicity, we will not take the spin of the particles into account. The following gives a duality between a Lieb-Thirring type bound and a lower bound for the kinetic energy of an N-particle fermion system. It is an immediate corollary of the Lieb-Thirring bound for $\gamma = 1$.

Theorem 1. *The following two bounds are equivalent for non-negative convex functions G and $F : \mathbb{R}_+ \to \mathbb{R}_+$ which are Legendre transformation of each other. The Lieb-Thirring bound:*

$$\sum_j |E_j| = \mathrm{tr}_{L^2(\mathbb{R}^d)}(H_0 + V)_- \leq \int G((V(x))_-) \, dx. \tag{15}$$

(*Usually with $H_0 = -\Delta$, but this does not matter in the following.*)
The Thomas-Fermi bound:

$$\langle \psi, \sum_{n=1}^N H_0 \psi \rangle_{\bigwedge^N L^2(\mathbb{R}^d)} \geq \int F(\rho_\psi(x)) \, dx, \tag{16}$$

for all antisymmetric states $\psi \in \bigwedge^N L^2(\mathbb{R}^d)$ with norm one. Here

$$\rho_\psi(x) := N \int_{R^{N-1}d} |\psi(x, x_2, \ldots, x_N)|^2 \, dx_2 \ldots dx_N$$

is the so-called one particle density associated with the antisymmetric N-particle state ψ.

For an explicit relation between F and G see (18) and (19).

Using the traditional Lieb-Thirring bound with $\gamma = 1$, one gets the following immediate

Corollary 2. *For normalized* $\psi \in \bigwedge^N L^2(\mathbb{R}^d)$,

$$\big\langle \psi, -\sum_{j=1}^N \Delta_j \psi \big\rangle_{L^2(\mathbb{R}^{Nd})} \geq C_{1,d}^{-2/d} K_d^{\mathrm{TF}} \int_{\mathbb{R}^d} \rho_\psi(x)^{\frac{d+2}{d}}\, dx$$

with

$$K_d^{\mathrm{TF}} = \frac{d}{d+2}\big(\frac{d+2}{2} L_{1,d}^{cl}\big)^{-2/d} = \frac{d}{d+2} \frac{4\pi^2}{\omega_d^{2/d}}.$$

On should note that the right hand side of this bound is exactly the Thomas-Fermi prediction for the kinetic energy of N fermions and K_d^{TF} is the Thomas-Fermi constant, see section 2.2. In particular, if $C_{1,d}$ is one, then the Thomas-Fermi ansatz for the kinetic energy, a priori only supposed to be asymptotically correct for large N, should be a true lower bound for all N. This is a situation very much similar in spirit to Pólya's conjecture.

Remark 3. Taking the spin of electrons into account, i.e., assuming that $\psi \in \bigwedge^N (L^2(\mathbb{R}^d, \mathbb{C}^q))$ is normalized (and $q = 2$ for real electrons) one has the lower bound

$$\langle \psi, \sum_{j=1}^N -\Delta_j \psi \rangle \geq (qC_{1,d})^{-2/d} K_d^{TF} \int \rho_\psi(x)^{(d+2)/d}\, dx. \tag{17}$$

Proof of Theorem 1: This proof is certainly known to the specialist, but we include it for completeness. In fact, the reverse implication is the easy one, (15) $\Leftarrow$ (16):
Fix $N \in \mathbb{N}$ and let $E_1 < E_2 \leq \cdots \leq E_N \leq 0$ be the first N negative eigenvalues of the one-particle Schrödinger operator $H = H_0 + V$. Usually, $H_0 = -\Delta$, but this does not really matter. By the min-max principle, we can assume without loss of generality that V is non-positive, $V = -V_- = -U$. If H has only $J < N$ negative eigenvalues, then we put $E_j = 0$ for $j = J+1, \dots, N$.

Consider $H_N = \sum_{j=1}^N (H_{0,j} - U(x_j))$ on $\bigwedge^N L^2(\mathbb{R}^d)$ be the sum of N independent copies of H (more precisely, one should write $H_N = \sum_{j=1}^N H_j$ with $H_j = \underbrace{\mathbf{1} \times \cdots \times \mathbf{1}}_{j \text{ times}} \times H \times \underbrace{\mathbf{1} \times \cdots \times \mathbf{1}}_{N-j-1 \text{ times}}$).

Let $\varphi_1, \dots, \varphi_N$ be the normalized eigenvectors corresponding to the eigenvalues E_j (if $J < N$ pick any orthonormal functions for $j > J$) and put

$$\psi := \varphi_1 \wedge \ldots \wedge \varphi_N \in \bigwedge^N L^2(\mathbb{R}^d),$$

the normalized antisymmetric tensor product of the φ_j's. Then

$$\begin{aligned}\sum_{n=1}^{N}|E_n| = -\sum_{n=1}^{N}E_n = -\langle\psi, \sum_{n=1}^{N}H_n\psi\rangle \\ = -\langle\psi, \sum_{n=1}^{N}H_0\psi\rangle + \langle\psi, \sum_{n=1}^{N}U_n\psi\rangle.\end{aligned}$$

Since $\sum_{n=1}^{N}U_n$ is a sum of one-body (multiplication) operators, we have $\langle\psi, \sum_{n=1}^{N}U_n\psi\rangle = \int U(x)\rho_\psi(x)\,dx$, by the definition of the one-particle density. Thus, taking (16) into account one gets

$$\begin{aligned}\sum_{n=1}^{N}|E_n| &\leq \int U(x)\rho_\psi(x)\,dx - \int F(\rho_\psi(x))\,dx \\ &= \int (U(x)\rho_\psi(x)\,dx - F(\rho_\psi(x)))\,dx \\ &\leq \int \sup_{t\geq 0}(U(x)t - F(t))\,dx = \int G(U(x))\,dx\end{aligned}$$

where we were forced to put

$$G(s) := \sup_{t\geq 0}(st - F(t)) \tag{18}$$

since we only know that $\rho_\psi(x) \geq 0$.

(15) $\Rightarrow$ (16): This is certainly standard, the argument in the original case goes through nearly without change. By min-max and the Lieb-Thirring inequality (15), we know that for any non-negative function U and any normalized antisymmetric N-particle ψ,

$$\langle\psi, \sum_{n=1}^{N}(H_0 - U)\psi\rangle \geq -\operatorname{tr}(H_0 - U)_- \geq -\int G(U(x))\,dx.$$

Thus

$$\begin{aligned}\langle\psi, \sum_{n=1}^{N}H_0\psi\rangle &\geq \langle\psi \sum_{n=1}^{N}U_n\psi\rangle - \int G(U(x))\,dx \\ &= \int U(x)\rho_\psi(x)\,dx - \int G(U(x))\,dx \\ &= \int \big[U(x)\rho_\psi(x) - G(U(x))\big]\,dx\end{aligned}$$

again by the definition of the one-particle density. Hence

$$\begin{aligned}\langle\psi,\sum_{n=1}^{N} H_0\psi\rangle &\geq \sup_{U\geq 0}\int \big[U(x)\rho_\psi(x) - G(U(x))\big]\,dx \\ &= \int \sup_{U(x)\geq 0} \big[U(x)\rho_\psi(x) - G(U(x))\big]\,dx \\ &= \int \sup_{s\geq 0} \big[s\rho_\psi(x) - G(s)\big]\,dx = \int F(\rho_\psi(x))\,dx,\end{aligned}$$

where, of course, we put

$$F(t) := \sup_{s\geq 0}(st - G(s)). \tag{19}$$

□

Remark 4. Since F and G are Legendre transforms of each other and since the double Legendre transform of a convex function reproduces the function (under suitable semi-continuity and convexity assumptions), we see that the Lieb-Thirring type inequality (15) and the Thomas-Fermi type kinetic energy bound (16) are dual to each other. In particular, one implies the other with the corresponding optimal constants. This could be interesting in the hunt for sharp constants, since Eden and Foias gave in [35] a direct and rather simple proof of the kinetic energy lower bound in one dimension.

Following Lieb and Thirring, the bound in Theorem 1 has a beautiful application to the Stability-of-Matter problem which we will discuss a little bit in section 2.3.

The Lieb-Thirring inequalities also found other applications, especially in the theory of non-linear evolution equations, as a tool to bound the dimension of attractors [28, 53, 57, 98, 131, 162].

1.6. **Classical results for the Lieb-Thirring constants.** The moment inequalities due to Lieb and Thirring are an important tool in the theory of Schrödinger operators since they connect a purely quantum mechanical quantity with its classical counterpart. Moreover, as we saw already, a dual version of it, the Sobolev inequality for fermions, is related to the theory of bulk matter. So a good understanding of the Lieb-Thirring coefficients is of some importance for our understanding of quantum mechanics.

In general dimensions $d \in \mathbb{N}$ one now knows the following properties of $C_{\gamma,d}$:

- $C_{\gamma,d} \geq 1$, which follows from the Weyl-asymptotic.
- Monotonicity in γ: $C_{\gamma,d} \leq C_{\gamma_0,d}$ for all $\gamma \geq \gamma_0$ (Aizenman and Lieb [2]).